DIFFERENCE SCHEMES OF IMPROVED ACCURACY FOR THE NUMERICAL SOLUTION OF SOME PROBLEMS IN AERODYNAMICS

A. I. Tolstykh

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16. Abstract

A procedure is proposed for developing third-order implicit conservative difference schemes for calculating viscid and inviscid gas flows. The approximation accuracy and stability of these schemes are analyzed. The flow of an ideal gas behind the detached shock wave at a blunt body is calculated as an example.

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DIFFERENCE SCHEMES OF IMPROVED ACCURACY FOR THE NUMERICAL SOLUTION OF SOME PROBLEMS IN AERODYNAMICS

A. I. Tolstykh

1. As a rule, in the numerical investigation of different flow classes, use is made of schemes either of first, or second order of accuracy for smooth functions of the initial equations. However, often it is desirable to use schemes of higher order of accuracy. This necessity arises, above all, when calculating viscid-gas flows when the error of approximation of the inertial terms can be comparable with the terms containing the coefficient of viscosity. More exact schemes can prove effective also in the calculation of flows of an ideal gas. Here the desired accuracy can be attained with relatively large steps of the calculation mesh.

The article /1/ shows methods of constructing conservative difference schemes up to the third order of approximation for all variables. Some are used for the numerical solution of the Navier-Stokes equations of a compressible gas. Below we examine problems associated with the approximation and stability of these schemes and, as an example, results of calculation of the flow of an ideal gas behind a detached shock wave in front of a blunt body are presented.

2. To construct schemes of third-order of approximation for the simplest equation

$$\frac{df(u, x)}{dx} + g(u, x) = 0, \qquad (1)$$

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* Numbers in the margin indicate pagination in the foreign text.

let us apply operators $A_+^{(i)}$ and $A_-^{(i)}$ on the mesh $x_i = ih$ by the formulas /37

$$\int_{x_i}^{x_{i+1}} f(x)\,dx = h\left(\frac{5}{12}f_i + \frac{8}{12}f_{i+1} - \frac{1}{12}f_{i+2}\right) + O(h^4) = h(A_+^{(0)}F)_{i+\frac{1}{2}} + O(h^4),$$

$$\int_{x_i}^{x_{i+1}} f(x)\,dx = h\left(\frac{5}{12}f_{i+1} + \frac{8}{12}f_i - \frac{1}{12}f_{i-1}\right) + O(h^4) = h(A_-^{(0)}F)_{i+\frac{1}{2}} + O(h^4). \qquad (2)$$

We can write the difference schemes for Eq. (1) in the form

$$\frac{\Delta_+^{(0)}f_i}{h} + (A_-^{(1)}g)_{i+\frac{1}{2}} = 0, \qquad (3a)$$

$$\frac{\Delta_-^{(0)}f_i}{h} + (A_+^{(0)}g)_{i+\frac{1}{2}} = 0, \qquad (3b)$$

$$\frac{\Delta_-^{(0)}f_i}{h} + (A_-^{(1)}g)_{i-\frac{1}{2}} = 0, \qquad (3c)$$

where

$$\Delta_+^{(0)}f_i = f_{i+1} - f_i, \quad \Delta_-^{(0)}f_i = f_i - f_{i-1}.$$

Substituting in (3a) - (3c) sufficiently smooth functions of f and g and expanding them in a Taylor series, for example, in the neighborhood of the points x /illegible/ and x /illegible/, for the error of approximation with Eqs. (1) we thus get the expressions

$$\frac{h^2}{24}\frac{d^2}{dx^2}\left(\frac{df}{dx} + g\right)_{i+\frac{1}{2}} + O(h^4),$$

$$\frac{h}{2}\frac{d}{dx}\left(\frac{df}{dx} + g\right)_i + \frac{h^2}{6}\frac{d^2}{dx^2}\left(\frac{df}{dx} + g\right)_i + O(h^3),$$

$$\frac{h}{2}\frac{d}{dx}\left(\frac{df}{dx} + g\right)_i + \frac{h^2}{6}\frac{d^2}{dx^2}\left(\frac{df}{dx} + g\right)_i + O(h^3).$$

By virtue of (1), all expressions in the parentheses and the derivatives of these expressions disappear so that the schemes (3a) - (3c) approximate Eq. (1) with the third order of accuracy for smooth solutions of the latter. Note that schemes (3b) and (3c) were separated from the set of schemes (3a) in order to find the nature of the approximation at node x_i.

For the equation

$$\frac{\partial f(u, x, y)}{\partial x} + \frac{\partial \varphi(u, x, y)}{\partial y} + \psi(u, x, y) = 0 \qquad (4)$$

at the mesh $x_i = ih$, $y_j = j_\ell$ we can get an approximation of the form $O(h^3 + \ell^k)$ by replacing the derivative $\partial\phi/\partial y$ when $x = x_i$ by any difference ratio $(\partial\phi/\partial y)$ with order of accuracy k and by using the operators $\Delta_{\mp}^{(i)}$ and $A_{\mp}^{(i)}$, respectively, to f_{ij} and $(\partial\phi/\partial y)_{ij} + \phi_{ij}$. In this case schemes (3) can be written as /38

$$\begin{aligned} &\frac{\Delta_{\mp}^{(i)} f_{ij}}{h} h + \left(A^{(i)}\left((\partial\varphi/\partial y) + \psi\right)\right)_{i+\frac{1}{2}, j} = 0, \\ &\frac{\Delta_{\mp}^{(i)} f_{ij}}{h} + \left(A^{(i)}\left((\partial\varphi/\partial y) + \psi\right)\right)_{i\pm\frac{1}{2}, j} = 0, \end{aligned} \qquad (5)$$

and the approximation errors, for example, in the case of scheme (3b) will be of the form

$$-\frac{h}{2}\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial x} - \frac{\partial\varphi}{\partial y} + \psi\right)_{ij} + \frac{h^2}{6}\frac{\partial^2}{\partial x^2}\left(\frac{\partial f}{\partial x} + \frac{\partial\varphi}{\partial y} + \psi\right)_{ij} + O(h^3 + l^k).$$

We can use the following two- or three-point formulas as the simplest expressions for $(\partial\phi/\partial y)$:

$$(\partial\varphi/\partial y)_{ij} = \frac{\varphi_{ij} - \varphi_{i,j-1}}{l} + O(l), \qquad (6a)$$

$$(\sigma_{\bar{x}}\,\partial y)_{ij} = \frac{3\bar{\varphi}_{ij} - 4\bar{\varphi}_{i,j-1} + \bar{\varphi}_{i,j-2}}{2l} + O(l^2) \qquad (6b)$$

This "nonuniform" approximation in all variables is meaningful also in those cases when it is desirable to have a high order of accuracy in one of the directions, for example, along the normal to the body in the case of viscid flows, while for other directions this is not as essential.

To approximate Eq. (4) with a third order of accuracy in all variables, let us use the operators $A_{\mp}^{(i)}$, $\Delta_{\mp}^{(i)}$ and $A^{(j)}$, and $\Delta^{(j)}$ corresponding to coordinates x and y, then we can write one of the sets of the resulting schemes, for example, as

$$\frac{(A_{+}^{(i)}(\Delta_{+}^{(i)} f))_{i,j-\frac{1}{2}}}{h} - \frac{(A_{-}^{(i)}(\Delta_{-}^{(i)}\bar{\varphi}))_{i+\frac{1}{2},j}}{l} + (A_{-}^{(j)}(A_{-}^{(j)}\bar{\varphi}))_{i+\frac{1}{2},j-\frac{1}{2}} = 0. \qquad (7)$$

Expanding sufficiently smooth functions of f and ϕ in a Taylor series in the neighborhood of the point i + ½, j, for the approximation error we get an expression of the form

$$\frac{l}{2}\frac{\partial}{\partial y}\left(\frac{\partial f}{\partial x} + \frac{\partial \bar{\varphi}}{\partial y} + \bar{\varphi}\right)_{i+\frac{1}{2},j} + \frac{l^2}{6}\frac{\partial^2}{\partial y^2}\left(\frac{\partial f}{\partial x} + \frac{\partial \bar{\varphi}}{\partial y} + \bar{\varphi}\right)_{i+\frac{1}{2},j} + \frac{h^2}{24}\frac{\partial^2}{\partial x^2}\left(\frac{\partial f}{\partial x} + \frac{\partial \bar{\varphi}}{\partial y} + \bar{\varphi}\right)_{i+\frac{1}{2},j} + O(h^3 + l^3),$$

which for f, ϕ, and Ψ satisfying Eq. (4) yields terms of the order of $O(h^3 + \ell^3)$.

Schemes of third-order accuracy in all variables plotted based on the concepts of the Runge-Kutta method were examined in /2/ and /3/. A large number of template /mesh/ nodes for each spatial variable evidently complicates their use in solving boundary value problems.

Note that schemes (3), (5), and (7) can be obtained by another approach, by passing the corresponding differential equations. To do this, it suffices to set up a balance of flows across the boundaries of elementary cells by using the quadrature formulas (2).

The conservativeness of the schemes described above evidently /39 permits their use also in describing discontinuity solutions of the starting equations (for example, in calculating flows of an ideal gas by shock waves).

To approximate the second-order equation written in the divergent form (for example, in problems of viscid flow), one can use the above-described method of constructing difference schemes, either by reducing this equation to a system of first-order equations, or by considering the expressions for flows through the corresponding boundaries of cells as dependent on the first derivatives of the functions being sought.

In particular, for the simplest equation is

$$\frac{\partial f(u, x)}{\partial x} - g(u, x) = \varepsilon \frac{\partial^2 u}{\partial x^2}, \qquad (8)$$

/illegible/ $f = f$ /illegible/ $- z\,(\partial u/\partial x)$, approximating the derivative with a second order of accuracy and using schemes (3), we get an approximation for the solution (8) of the form $O(\max(zh^2, h^3))$, so that for small ε, at least in the domain of weak gradients of function u, gives a practically high degree of accuracy.

3. When schemes (5) - (7) were used in solving boundary value problems, the problem of selecting operator A_+ or A_- arises. This selection can be based on the following considerations: first, the mesh nodes used must not exceed the bounds of the domain under consideration and, secondly, the scheme must be stable at least in the linear approximation for Cauchy's problem.

To revise the last requirement, let us investigate the stability of schemes (5) - (7) as applied to the simplest linear equation:

$$\frac{\partial u}{\partial t} = a\frac{\partial u}{\partial x}, \quad a = \text{const.} \tag{9}$$

Let us first consider in the mesh $t_m = m\tau$, $x_n = nh$ the approximation (5) and (6a), which, for example, when $a > 0$ can be written as

$$\frac{5}{12}\frac{u_{n+1}^{m+1} - u_{n+1}^{m}}{\tau} + \frac{8}{12}\frac{u_n^{m+1} - u_n^m}{\tau} - \frac{1}{12}\frac{u_{n-1}^{m+1} - u_{n-1}^m}{\tau} = a\frac{u_{n-1}^{m+1} - u_n^{m+1}}{h} \tag{10}$$

Seeking the proper function of the operator for converting from the m-th layer to the (m + 1)-th layer in the form $u_n = e^{i\alpha a}$, for the modulo of the proper number λ we get the expression

$$|\lambda|^2 = \frac{1}{(1 - ar\,\mathrm{Re}\,W_k)^2 - (\mathrm{Im}\,W_k)^2}, \tag{11}$$

where k here and in the following is minus or plus; $r = \tau/g$; W_- and W_+ are functions of the complex argument corresponding to operators $A_-^{(n)}$ and $A_+^{(n)}$:

$$W_- = \frac{e^{i\alpha} - 1}{\frac{5}{12}e^{i\alpha} + \frac{8}{12} - \frac{1}{12}e^{-i\alpha}}, \quad W_+ = \frac{e^{i\alpha} - 1}{\frac{5}{12} + \frac{8}{12}e^{i\alpha} - \frac{1}{12}e^{2i\alpha}}.$$

We can easily see that $\mathrm{Re}\,W_- \leqslant 0$ and $\mathrm{Re}\,W_+ \geqslant 0$, so that for operator $A_k^{(n)}$ ensuring that the inequality $a\,\mathrm{Re}\,W_k \leqslant 0$ is satisfied, schemes (5) and (6a) are absolutely stable. /40

In the case of the approximation (5) and (6b), and also schemes of the third order of accuracy, of type (7), expressions for the proper number λ take on the form

$$S(r)\ ar\,W_k = 0, \quad S(r) = \frac{3}{2}r^2 + \frac{1}{2}r, \tag{12a}$$

$$1 - R(r)\,ar\,W_k = 0, \quad R(r) = \frac{5}{12}r^2 + \frac{8}{12}r - \frac{1}{12}. \tag{12b}$$

Obviously, to satisfy the relation $|\lambda| \leqslant 1$, it is also necessary to satisfy the condition a Re $W_k \leqslant 0$. To verify the sufficiency of the latter, the values of λ were computed for different arguments $\alpha(0 \leqslant \alpha \leqslant 2\pi)$ and the parameter $|a|\ r$. Fig. 1 shows the variation in $A = \max |\lambda|$ with variation in $|a|\ r$

0/illegible/

for schemes (5), (6a), and (7). Clearly, when a Re $W_k \leqslant 0$, schemes (5) and (6a) are absolutely stable, while scheme (7) is provisionally stable (stable when $|a|\ r \leqslant 1$).

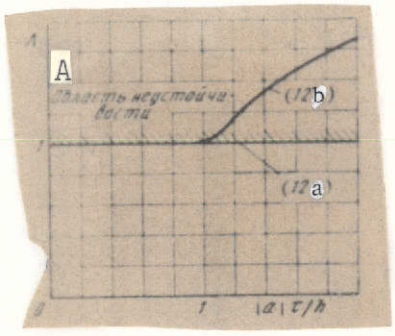

Fig. 1.

Key: A. Domain of instability

In the case of the second-order equation of the form

$$\frac{\partial u}{\partial t} = a\frac{\partial u}{\partial x} + \nu\frac{\partial^2 u}{\partial x^2} \qquad (13)$$

schemes (5) - (7) for derivatives of the first order with appropriate approximation of the derivative $\partial^2 u/\partial x^2$ in the $(m + 1)$-th time layer when a Re $W_k \leqslant 0$, absolutely stable implicit schemes are formed.

When the difference schemes (5) - (7) are used for equations in gas dynamics, an estimate of the stability necessary to select the zero indices of the operators used can be obtained from the difference equations for the corresponding "nondivergent" scheme with "frozen" coefficients. Let us examine as a simple example the schemes (5) and (6b) for one-dimensional nonsteady equations in gas dynamics written in Euler's variables in the form

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0, \quad \frac{\partial \rho u}{\partial t} + \frac{\partial (\rho u^2 + p)}{\partial x} = 0,$$
$$\frac{\partial}{\partial x}\left(\frac{h}{\gamma} + \frac{u^2}{2}\right) + \frac{\partial u\left(h + \frac{u^2}{2}\right)}{\partial x} = 0, \quad p = \frac{\gamma - 1}{\gamma}\rho h, \qquad (14)$$

where u, ρ, p, h, and γ are velocity, density, pressure, enthalpy, and adiabatic index, respectively.

Let the condition $|u| \geqslant c = (\gamma - 1)h$ be satisfied in some region, and then by introducing in the mesh $t_m = m\tau$, $x_n = n\hat{o}$ the operator $A_k^{(n)}$ so that u Re $W_k \geqslant 0$, we get for the proper number λ of the operator for converting to the next time layer an equation of the form

$$[S(\lambda) + uW_k r]\,[[S(\lambda) + uW_k r]^2 - c^2 W_k^2 r^2] = 0,$$

where $r = \tau\hat{o}$, and $S(\lambda)$ is a function determined in Eq. (12a). /41
This equation breaks down into three equations of the form (12a) with coefficients $a = -u$, and $a = -(u + c)$, each of which, λ according to the preceding results, determines the values of not exceeding unity modulowise.

In the domains where $|u| < c$, in approximations of the first and second equations in system (14), let us use the operator $A_k^{(n)}$, for which Re $W_k \geqslant 0$, and in the approximation of the second equation let us change the sign in the selected subscript by the opposite sign. Then noting that Im W /illegible/ Im W_-, we get the following equations for determining λ values:

$$S(\lambda) + uW_k r = 0,$$
$$S^2(\lambda) + 2ur(\operatorname{Im} W_k)S(\lambda) - |W_k|^2 r^2 (c^2 - u^2) = 0.$$

Examining the second of these equations as a quadratic equation in $S(\lambda)$, we arrive at two equations of the form (12a) with purely imaginary values of coefficient a ensuring that condition $|\lambda| \leqslant 1$ is satisfied. Thus, scheme (5) and (6b) for this method of approximating system (14) is absolutely stable in the approximation of "frozen" coefficients.

In solving systems of difference equations in cases when there is a transition from one layer to another, one can use the

fitting method. Let us examine, for simplicity, the case of a m mixed problem for Eq. (9) in the strip $0 \leqslant x \leqslant 1$:

$$u(x, 0) = \varphi(x), \quad u(1, t) = \psi(t) \quad (a > 0).$$

When scheme (5) and (6a) (a Re $W_- \leqslant 0$) is used, the difference equations can be written as

$$\left.\begin{aligned} u_{n+1}^{m+1}\left(ar - \frac{5}{12}\right) - u_n^{m+1}\left(ar + \frac{8}{12}\right) + \frac{1}{12} u_{n-1}^{m+1} = d_n \\ (n = 1, 2, \ldots, N-1), \quad u_N^m = \psi^{m+1}, \end{aligned}\right\} \tag{15}$$

where d_n signifies the terms containing the values of the functions at the m-th layer. The secondary boundary condition for (14) can be obtained from the system of two equations written with n = 1 and n = 2 with reference to a change in the index of the operator $A_k^{(n)}$ by the opposite sign. After canceling out u_0^{m+1}, we get the relation

$$u_1^{m+1} = \frac{\left(a^2 r^2 - \frac{1}{6}\right) u_2}{a^2 r^2 + ar + \frac{1}{3}} + k_1, \tag{16}$$

where k_1 denotes terms dependent on d_2 and d_1. Using the expressions for the fitting-in coefficients, we can show that Eq. (15), with condition (16), can realize the stable curve-fitting.

Note that an iterative method of solving system (15) is also possible, where the value u_{n-1}^{m+1} is taken from the preceding iteration and the equations are reduced to two-point equations; we can show that the proper numbers of the corresponding conversion operator are smaller than unity and the convergence condition has been satisfied. The use of the iterative process is meaningful in the case of nonlinear equations.

4. Let us examine briefly the problem of applying the above-described type of schemes to calculating the steady axi-symmetric flow of an ideal gas between a blunt body and a /42

detached shock wave. We will assume the surface of the shock wave to be the discontinuity surface at which Hugoniot's relation is satisfied. By selecting the system of coordinates sn associated with the body contour (coordinates s and n are directed, respectively, along the surface and along the normal to it) and by introducing the new variable $\xi = n/\varepsilon$ where ε is the distance of wave separation, let us write the equations of motion and continuity in the "divergent" form (4), assuming f and ϕ to be the following vectors:

$$\varphi = \left(\varepsilon \frac{\rho u^2 + p}{H}, \varepsilon \frac{\rho u v}{H}, \varepsilon \frac{\rho u}{H}\right),$$

$$f = (\rho v u, \rho \bar{v} v + p, \rho v).$$

Here u and v are the tangential and normal velocity components, $\bar{v}$ is some combination of u and v arising owing to the introduction of variable ξ, and H is the Lame coefficient. The role of coordinates x and y in (4) are played, respectively, by ξ and s. As the equations closing the system, we will use Bernoulli's integral, the equation of state, and the geometrical relation for the compression discontinuity expressing the relation between the quantity ε and the angle of inclination of the wave to the body. In the strip $0 \leqslant s \leqslant s_M$, $0 \leqslant \xi \leqslant 1$ /the point (0, 0) lies at the critical point of the body/ on the mesh $s_i = i\Delta s$, $\xi_j = j\Delta\xi$ ($i = 0, 1, \ldots, M$; $j = 0, 1, \ldots, N$), let us introduce the approximations (5) and (6b)[1] with $h = \Delta$ and $\ell = \Delta s$.

To solve the system of the difference equations, use was made of the iterative method with relaxation equivalent to some implicit scheme of the finite-difference method. By iteration we will mean the calculation of the entire flow field by an implicit scheme

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[1] The derivative $\partial p/\partial s$ was approximated by means of central differences.

analogous to scheme (10) for the evolutionary equation (9); here the role of the time variable t is played by the coordinate s ($s = 0, \Delta s, \ldots, M\Delta s$). The final transition to the next (m + 1)-th iteration for any function F was carried out by the formula

$$F_{ij}^{(m+1)} = (1 - \omega) F_{ij}^{(m)} + \omega \bar{F}_{ij}^{(m+1)},$$

where $\bar{F}_{ij}^{(m+1)}$ is the value found by solving the difference equations, and ε is the relaxation parameter. Both the "simultaneous" as well as "successive" relaxation were employed for different calculation variants; in the latter case the values of the function were relaxed immediately after they were determined at all points of the arc $s = s_i$.

Successive computation of the unknown functions in passing from one ray to another can be realized in different ways. The following procedure was used: the general system of difference equations was divided into subsystems corresponding to each differential equation; in each of these subsystems several gas-dynamic functions were assumed to be known, that is, they were taken either from the preceding iteration, or else from the solutions of other subsystems found during the current iteration. For example, in the difference equations corresponding to the /43
equation of motion in a projection onto the s axis, the values of the velocity u_{ij} were assumed unknown, while all the remaining functions ρ_{ij}, v_{ij}, and h_{ij} were assumed to be known. The values thus found in the entire field after relaxation were used in the remaining equations, and so on.

The specific details of solving the difference equations along the rays s = const amount to the following. The values of the functions multiplied by the coefficient 1.12 were assumed known from the preceding "internal" iteration for each ray so that the three-point difference equations reduced to two-point equations.

This made it possible to conduct a "running computation" from the wave or from the body with subsequent internal interations. In practice, sometimes it was sufficient in general not to iterate the values of the functions on the ray, but to take the quantities transferred to the right-hand side of the equations from the preceding "external" iteration.

The difference equations approximating the equation of motion in the projection onto the s axis were regarded as quadratic in values of the velocity u_{ij} and were solved successively from wave to body.

The continuity and motion equations in projections onto the n axis were assumed to be linear, respectively in velocity v and density ρ. The values of v_{ij} were determined successively from body to wave, while the values r_{ij} were determined from wave to body; the value of the detachment ε was found from the difference approximation of the continuity equation.

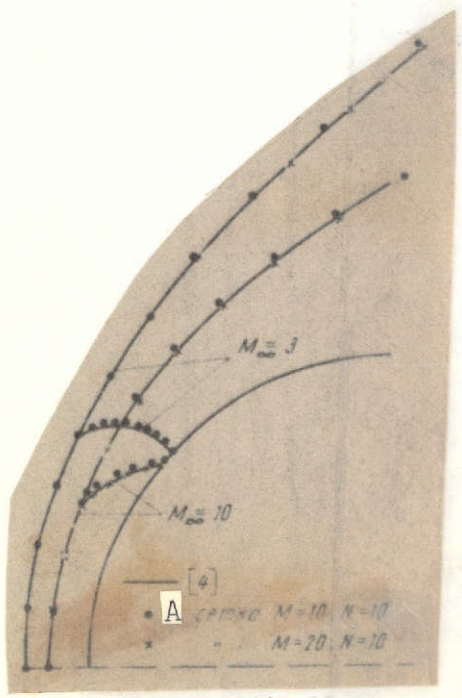

Fig. 2.
Key: A. Mesh

The values of the functions calculated at the i-th ray were used in the difference equations for the (i + 1)-th ray. The conditions of symmetry and the derivatives $(\partial u/\partial s)_{s=0}$ calculated from the preceding iteration were used at the ray s = 0; when $s = s_1$, two-point difference approximations of derivatives in s were used always, without loss of accuracy owing to the symmetry conditions; these derivatives were written along the ray $s = s_M$ by means of the left difference ratios.

Selection of operators $A_+^{(j)}$ or $A_-^{(j)}$, if this selection influenced

the stability of the scheme in the linear approximation, was carried out just as in the case of equation (9), with the only difference that instead of (9), we considered the "nondivergent" equations with "frozen" coefficients with the corresponding independent equations or systems. Selection of the subscript k of operator $A_k^{(j)}$ to some degree is analogous with the selection of the direction of the nonsymmetric differences as a function of the signs of velocities in nonsymmetric difference schemes; here, in view of the nonlinearity of the equations the final conclusion as to the stability of the approximation used can be made only after numerical experiments.

The calculations were conducted for values of the relaxation parameter $\omega = 0.1$; and the number of iterations to obtain three coincident values of the numbers over the last 50 iterations was 200-300. /44

As an example, in Fig. 2 are shown the positions of the shockwave and the sonic line for the $M_\infty = 3$ and 10 and the adiabatic index $\gamma = 1.4$ calculated for several difference meshes ($s_M = 1.6$); also given there are the data from [4]. In Fig. 3 is shown the distribution of pressure along the body contour compared with the results in [4].

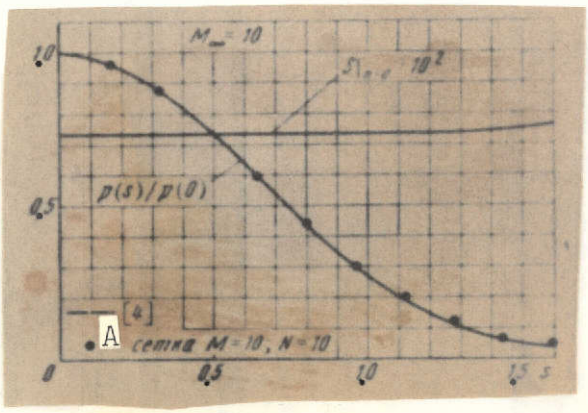

Fig. 3.

Key: A. Mesh

As we can see from Figs. 2 and 3, the data are quite close to the generally accepted results and differ little with increase in step Δs. For control of the calculation accuracy, we can use the value of the entropy $S = p/\rho^\tau$ at the zero streamline, since the equation of conservation of entropy was never used in the initial system.

Fig. 3 gives the function of S(s) varying over the interval [0, $\pi/2$] by not more than 4 percent.

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